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REACTION DYNAMICS ON SEMICONDUCTOR SURFACES(U)  
RENSSELAER POLYTECHNIC INST TROY NY DEPT OF MATERIALS  
ENGINEERING J B HUDSON 28 FEB 88 N00014-86-K-0259

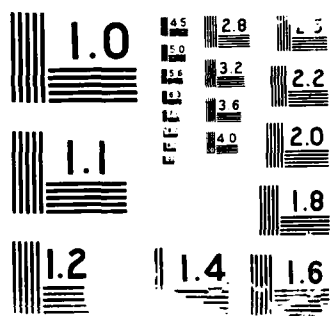
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FINAL REPORT

REACTION DYNAMICS ON SEMICONDUCTOR SURFACES

by

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# ABSTRACT

The combined techniques of molecular beam relaxation spectroscopy and Auger electron spectroscopy have been used to study the reactions of  $H_2$  and  $O_2$  on clean iron surfaces and of Kr,  $H_2$  and  $O_2$  on clean silicon and germanium surfaces. Results include adsorption and permeation of H in iron,  $H_2O$  formation on iron, oxidation of iron, volatilization of silicon and germanium in oxygen, krypton physisorption on germanium and H adsorption on silicon.

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## I. DESCRIPTION OF PROJECT

In this program, a range of surface analytical techniques, including Auger electron spectrometry (AES), molecular beam relaxation spectroscopy (MBRS) and thermal desorption spectroscopy (TDS), were used to study the dynamics of chemical reactions on surfaces. Information obtained includes the rate of formation of adsorbed or product species, the extent of surface coverage by reaction products or intermediates, the surface reaction mechanism and the rate constants for the various unit reaction steps. This information has been used to deduce the energetics and kinetics of adsorption of gases on metal and semiconductor surfaces, the kinetics of a bimolecular surface reaction on a metal surface, and the kinetics of volatilization reactions on semiconductor surfaces.

## II. SUMMARY OF RESULTS OBTAINED

The results obtained during the contract period fall into two groups: Adsorption and reaction of gases on iron surfaces and adsorption and reaction of oxygen on silicon and germanium surfaces.

The studies on iron were begun during a previous contract period. Efforts during the current period were concentrated on interpretation of previously collected data and preparation of the resulting conclusions for publication. These results are described in Technical Reports Number 1-7, and have been published as papers 1-7 in the section on Publications.

The experimental work carried out during the present contract period involved the use of molecular beam scattering of various gases from Si(100) and Ge(100) surfaces to determine the reaction mechanisms involved. Progress to date is summarized below:

A. Hydrogen on Si(100): An attempt was made to determine hydrogen adsorption kinetics on silicon using an  $H_2$  molecular beam. The experiment yielded a null

result. The activation energy for dissociative adsorption is apparently too high to be surmounted at the available beam energy and surface temperature. This project is currently in abeyance until an atomic hydrogen beam source can be developed.

B. Oxygen on Si(100): The interaction between an  $O_2$  molecular beam and a Si(100) surface was studied by both AES and MBRS. The uptake rate at low temperature, as measured by AES, was consistent with the results obtained by other (1,2). MBRS studies were abandoned when we became aware of published results by two other groups using similar techniques (1,2).

C. Krypton on Ge(100): This preliminary study was carried out to test a previously-developed deconvolution technique for the analysis of MBRS data. Analysis of these data is currently in progress.

D. Oxygen Ge(100): In this study, we are using MBRS and TDS to characterize the reaction of  $O_2$  with Ge(100). Both static dosing and molecular beam dosing are being used, with mass spectrometric detection. Results to date indicate that the oxygen adsorption process has an activation barrier in the entry channel. We is continuing under alternate sponsorship to complete this project.

### III TECHNICAL REPORTS

1. The Influence of Desorption Kinetics on Hydrogen Permeation in Iron, M. Arbab and J. B. Hudson, 7/30/87

2. The Adsorption of  $H_2$  and  $D_2$  on Fe(110) I: Helium Scattering as a Probe of Adsorption, E. A. Kurz and J. B. Hudson, 7/30/87.

3. The Adsorption of  $H_2$  and  $D_2$  on Fe(110) II: Angle Resolved Thermal Desorption Spectroscopy and Kinetic Mechanism, E. A. Kurz and J. B. Hudson, 7/30/87.

4. The Adsorption of  $H_2$  and  $D_2$  on Fe(110)-Kinetics and Energetics, E. A. Kurz and J. B. Hudson, 2/28/88.
5. The Reaction of Hydrogen with Oxygen on a Polycrystalline Iron Surface, M. Arbab and J. B. Hudson, 2/28/88.
6. The Kinetics and Mechanism of Oxygen Uptake on a Polycrystalline Iron Surface, M. Arbab and J. B. Hudson, 2/28/88.
7. The Titration of Oxygen on a Polycrystalline Iron Surface by Permeating Hydrogen, M. Arbab and J. B. Hudson, 2/28/88.

#### IV PUBLICATIONS

1. The Influence of Desorption Kinetics on Hydrogen Permeation in Iron, M. Arbab and J. B. Hudson, Applied Surface Sci. 29, 1, (1987).
2. The Adsorption of  $H_2$  and  $D_2$  on Fe(110) I: Helium Scattering as a Probe of Adsorption, E. A. Kurz and J. B. Hudson, Surface Sci. 195, 15 (1988).
3. The Adsorption of  $H_2$  and  $D_2$  on Fe(110) II: Angle Resolved Thermal Desorption Spectroscopy and Kinetic Mechanism, E. A. Kurz and J. B. Hudson, Surface Sci. 195, 31, (1988).
4. Extended Abstract: The Adsorption of  $H_2$  and  $D_2$  on Fe(110) - Kinetics and Energetics, E. A. Kurz and J. B. Hudson, J. Vac. Sci. Technology (in press).
5. Extended Abstract: The Reaction of Hydrogen with Oxygen on a Polycrystalline Iron Surface, M. Arbab and J. B. Hudson, J. Vac. Sci. Technology (in press).
6. The Kinetics and Mechanism of Oxygen Uptake on a Polycrystalline Iron Surface, M. Arbab and J. B. Hudson, submitted to Surface Science.
7. The Titration of Oxygen on a Polycrystalline Iron Surface by Permeating Hydrogen, M. Arbab and J. B. Hudson, submitted to Surface Science.



## V. PERSONNEL

The following students received full or partial support as Research Assistant from this contract:

1. Edward A. Kurz. Dr. Kurz completed the requirements for the Ph.D. in Materials Science in August, 1986.
2. Mehran Arbab. Dr. Arbab completed the requirements for the Ph.D. in Materials Science in July, 1987.
3. Bing-Xi Sun. Ms. Sun is expected to complete the requirements for the Ph.D. in Physics during the 1988-89 Academic year.

## VI REFERENCES

1. M. L. Yu and B. N. Eldridge; Phys. Rev. Letters 58 169, (1987).
2. M. P. D'Evelyn, M. M. Nelson and T. Engel; Surface Sci 186, 75, (1987).

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